- **Polarized Beam Reduction Procedures**

beta version
2 FEB 2012
updated
5 OCT 2012
1 JUL 2013

These are the input panels to set and calculate polarization parameters necessary for the matrix corrections to the cross sections. There are 4 input panels to get the necessary information from the users and their use is described below:

To start:
1- Load the SANS Reduction package
2- Load the Polarization Reduction package (this also loads SANS reduction if you forget)
3- Pick Path on the main (yellow) panel to set the data path
4- Work through the panels IN ORDER. The panels are called up from the Macros Menu, and are numbered in the order that you need to populate them.
5- The "state" of any of the four panels can be saved/restored through the items on the Macros Menu. This is intended for users with the demo version of Igor, to avoid the need to re-enter run information.

The input panels are:

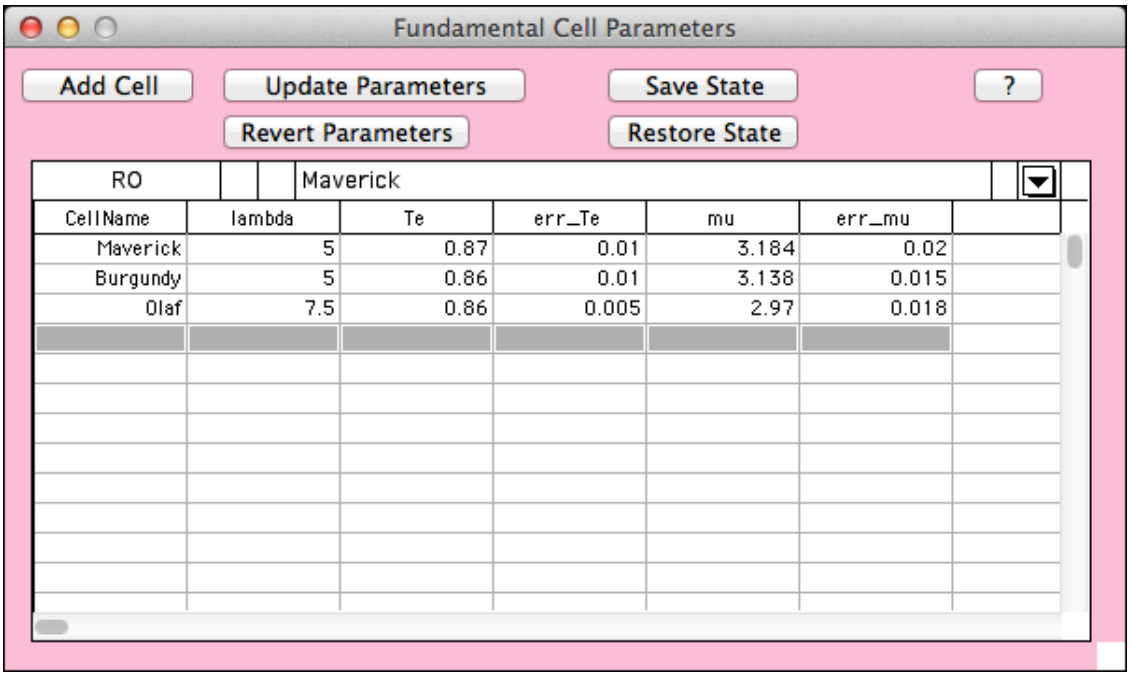
References:

K Krycka, W C Chen, J A Borchers, B B Maranville, S M Watson, "Polarization-analyzed small-angle neutron scattering. I. Polarized data reduction using Pol-Corr." *Journal of Applied Crystallography* (2012) **45** pp. 546-553.

K Krycka, J A Borchers, Y Ijiri, R Booth, S A Majetich, "Polarization-analyzed small-angle neutron scattering. II. Mathematical angular analysis." *Journal of Applied Crystallography* (2012) **45** pp. 554-565.

The first panel:

Fundamental Cell Parameters



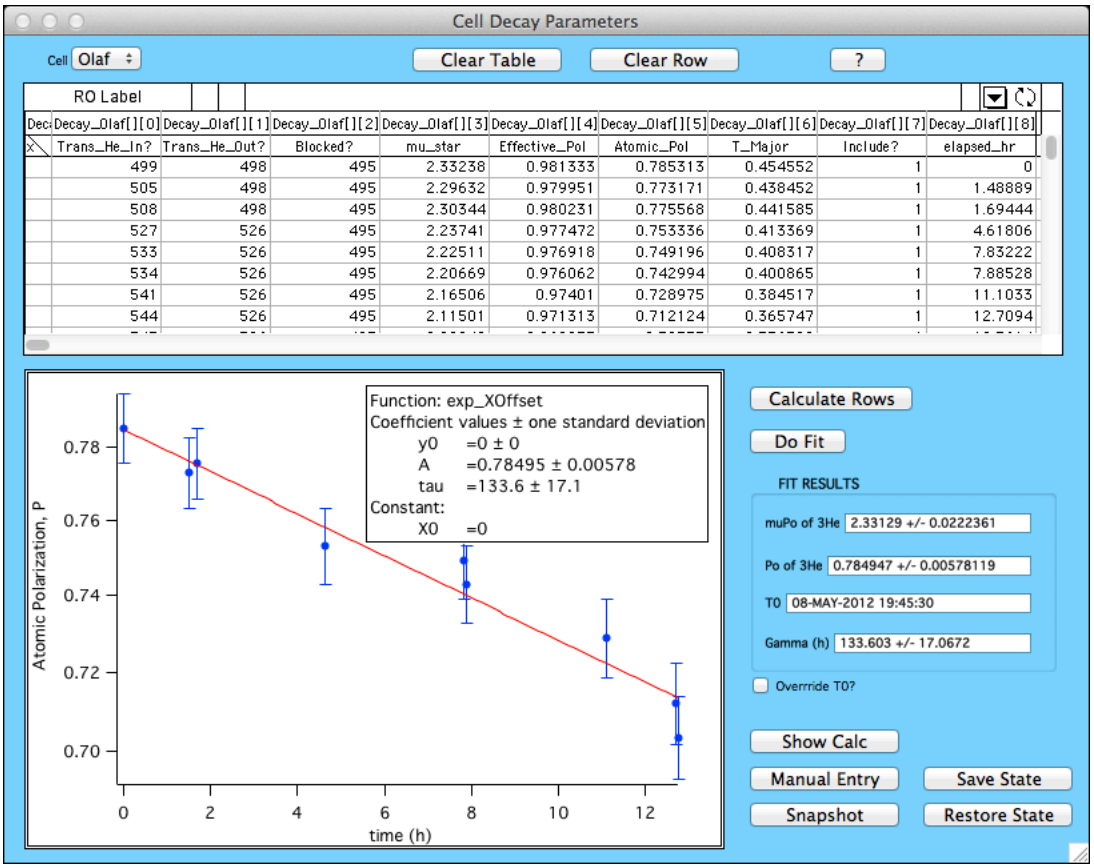
- Say <yes> to use the default parameters.
- The labels of the columns are pretty self-explanatory.
- If you change any of these parameters in the table, you MUST click "Update Parameters", or your changes won't be recognized by later calculations.
- "Revert" will discard ALL of your changes. So don't use this unless you've really messed up.
- If you want to add another cell, click "Add Cell" and you'll get a new row in the table. Fill it in and then be sure to "Save Parameters".
- NOTE: the changes are saved per experiment
- Save State / Restore State allows you to export all of the parameters that you have entered in the table. This is a necessary step to save your work with the demo version of Igor. With the full version, saving the experiment will save the table automatically.

Other tidbits:
- The default parameters are stored in the file Pol_PolarizationPanels.ipf
- On opening the panel, default cell parameters are loaded and in the folder root:Packages:NIST:Polarization:Cells
- important parameters are held in global key=value strings gCell_<name>
- cell names and parameters are used by the 2nd panel for calculation of the Decay constant

No math is done here. Previously measured values are simply input here for later calculations using a particular named cell.

The second panel:

Cell Decay Constant Panel



- Open the panel, and "pop" the selected cell from the top left popup menu. This will generate a table that you can then fill out. Even if you don't want to fill in the table, but rather use the Manual Entry - you still need to do this step to generate some necessary storage behind the scenes.
- The table is looking for run numbers - He in/out/blocked. These columns are titled with "?" at the end, looking for input from you. It is also looking for a "1" in the "Include?" column, to include the row in the calculation.
- Once those three run numbers are entered - then "Calculate Rows" will calculate everything on the table. Doesn't matter what you've selected. You may see error messages about how the data is at mismatched conditions. If they bother you, do something about it. Number of attenuators is automatically corrected. Other errors, not so.
- "Show Calc" will show the count rates for each of the files in a table, to show how the numbers were calculated. Not a necessary step to see this.
- With at least (3) rows populated, you can "Do fit" to fit the decay constant. Be sure that the column "Include" is populated with "1's" rather than zeros. If there are 1's present, the data is used in the fit, zeros are excluded.
- bad points can be excluded from the fit, and "Do fit" again to get (maybe) better results.
- Note that time=0 is taken from the file date stamp in the first row of the table. If you have a different time that you want to use as To, then check the box, and enter it in the T0 box in the format:

29-NOV-2010 14:24:00

- Manual entry allows you to enter the three decay parameters and their errors, and a run number that is to be used for T=0 of the decay. (This may change in the future to be entered as a date-time string instead)
- "Snapshot" will save the image of the panel to save the state of what you've got. You had better be saving the experiment too, unless you like starting over again from scratch.
- Save State / Restore State allows you to export all of the parameters that you have entered in the table. This is a necessary step to save your work with the demo version of Igor. With the full version, saving the experiment will save the table automatically.

Other tidbits:
- decay constant determined for each cell.
- popping the cell name makes 2 waves, Decay_<cellname> and DecayCalc_<cellname>
- Decay_ is the wave presented in the table. Specified transmission run numbers are entered and "Calc Sel Row" does the calculation of mu and Pcell (for all rows, actually)
- DimLabels are used for the arrays to make the column identity more readable than simply an index
- time=0 is taken from the first file, unless overridden
- Calculations are based on the count rate of the file, corrected for monitor and attenuation
- alerts are posted for files in any row that are not at the same attenuation or SDD
- if "include" column is == 1, that row will be included in the fit of the decay data
- excluded points are plotted in red
- results of the fit are printed on the panel, and written to the wave note of the Decay_ wave (not DecayCalc_) for use in the next panel
- manual entry of all of the parameters in the wave note is allowed.

The math that is done here is:

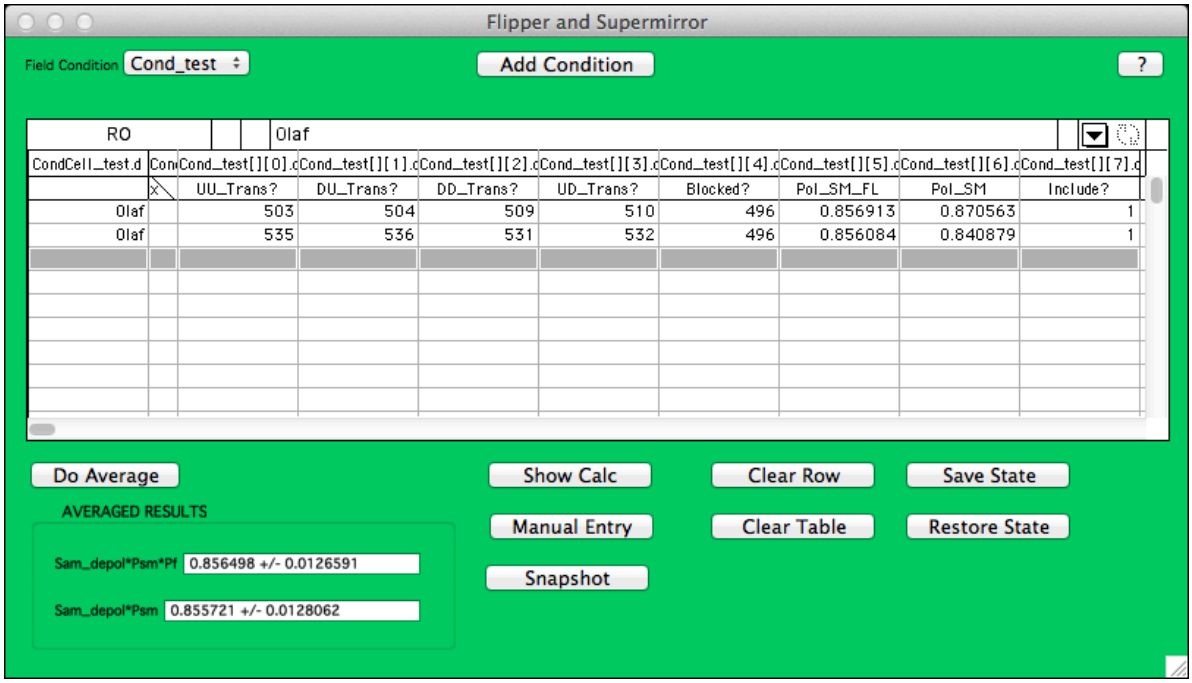
$$\mu\wp_{He} = a\cosh\left(\frac{T_{He,unpol} - T_{bkg}}{T_{Open,unpol} - T_{bkg}}\left(\frac{1}{T_e e^{-\mu}}\right)\right)$$

Then fitted to a decaying exponential to determine gamma and Po:

$$\mu\wp_{He} = P_0\, e^{-t/\Gamma}$$

The third panel:

Flipper States Panel



-This panel calculates the flipper and supermirror efficiencies for a given "condition". Note that this "condition" may have contributions from multiple cells.

- Start by clicking "Add Condition" and entering a condition name. Keep it short and to the point.
- "Pop" that new condition "Cond_" in the popup to get a table. If you want to manually enter the parameters and errors, you can do that now. Otherwise, you'll need to fill in the table.
- First - the cell name. type it in just as the cells named.
- Next the files. Self-explanatory column headings for the 5 files needed. Just the run numbers.
- Last - "Do Average" calculates the polarization for all of the entries on the table (ONLY those with "1's" in the include column) and puts the results on the panel.
- Save State / Restore State allows you to export all of the parameters that you have entered in the table. This is a necessary step to save your work with the demo version of Igor. With the full version, saving the experiment will save the table automatically.

Other tidbits:
- Waves Cond_<condition> and CondCalc_<condition>, and CondCell are created
- DimLabels are used for the arrays to make the column identity more readable than simply an index
- Enter the name of the cell in the first column (the cell must be defined and decay calculated)
- enter transmission run numbers as specified in the table

- Do Average will calculate the Psm and PsmPfl values (and errors) and average if more than one row of data is present (and included)
- results are printed on the panel, and written to the wave note of Cond_<condition>
- results are used in the calculation of the polarization matrix
- (the cell name is not entered using a contextual menu, since this is difficult for a subwindow)
- (the wave note no longer needs the cell name)

The math that is done here is:

$$P_{sm} = \frac{\left(\frac{T_{(\uparrow\uparrow)}(t_1) - T_{bkg}}{T_{(\uparrow\downarrow)}(t_2) - T_{bkg}} - 1\right)}{P_{cell}(t_1)\left(1 + \frac{T_{(\uparrow\uparrow)}(t_1) - T_{bkg}}{T_{(\uparrow\downarrow)}(t_2) - T_{bkg}}\right)}$$

and

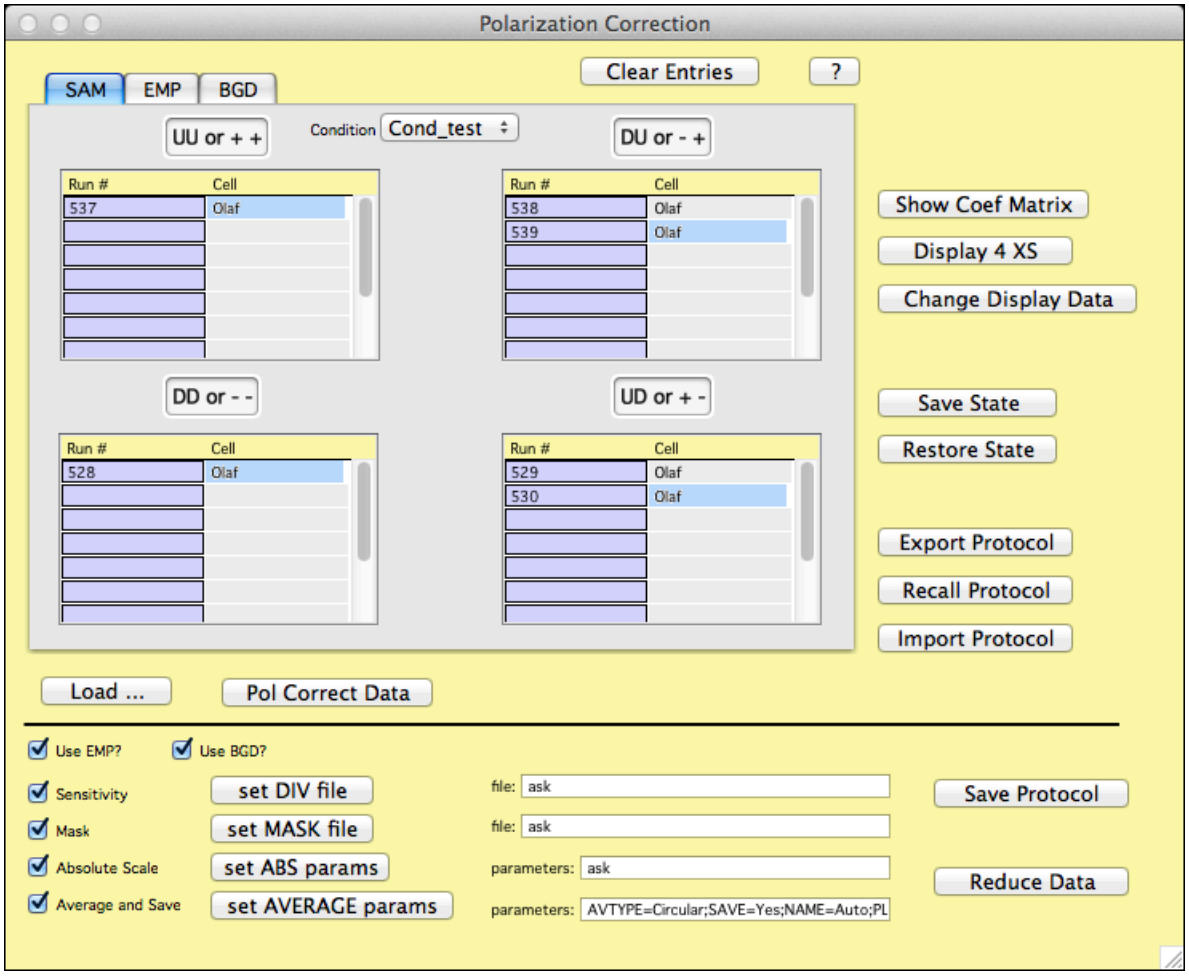
$$P_f P_{sm} = \frac{\left(\frac{T_{(\downarrow\downarrow)}(t_1) - T_{bkg}}{T_{(\downarrow\uparrow)}(t_2) - T_{bkg}} - 1\right)}{P_{cell}(t_1)\left(1 + \frac{T_{(\downarrow\downarrow)}(t_1) - T_{bkg}}{T_{(\downarrow\uparrow)}(t_2) - T_{bkg}}\right)}$$

where the polarization of the cell at any time t (after the start time, t0) is:

$$P_{cell}(t) = \tanh\left(\mu \wp_{He}(t_0)\, e^{-\Delta t/\Gamma}\right)$$

The fourth panel:

Polarization Correction Panel



This is the panel where all of the polarization correction and the data reduction is actually done. The appropriate runs are entered, at the specified flipper/field condition. Cells are entered specific to each run, while the flipper/field condition is for the entire set of SAM or EMP measurements. The field condition can be different for SAM and EMP measurements. Since no field condition is necessary for the BGD condition, none is entered. Last, a protocol is set up like usual, but with a few extra steps as noted to perform the polarization corrections.

The upper part of the panel has three tables, for SAM, EMP, and BGD files, plus a popup menu to define the flipper/field condition as defined in the (green) flipper panel of step 3. With a particular tab open, choose the field condition and enter the run numbers for each type of spin combination. Up to 10 runs can be entered for each spin combination.

- Enter the run numbers, then click in the cell column and pick the cell from the popup.
- The "Load..." button will load all of the files from the 4 states into the folder specified on the tab. If there are any errors - such a the cell not being specified, then you'll

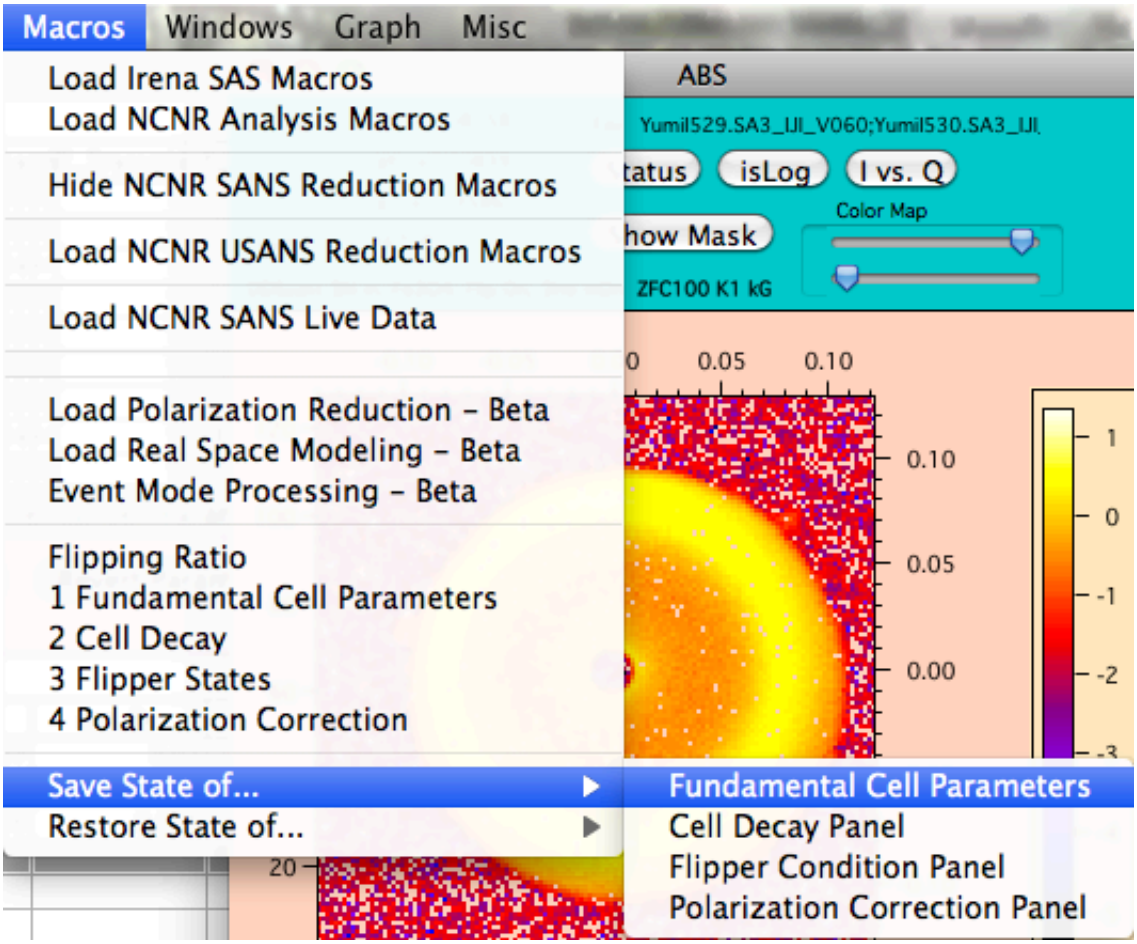
get a message and a chance to fix the errors.

- Then, "Pol Correct Data" will do the polarization correction on the data that was just loaded. This step must be done before the reduction protocol.
- "Show coef matrix" shows the 4x4 matrix used for the inversion of the data
- "Change displayed data" allows you to change the data that is displayed in the 2D SANS data window. This is needed to be able to see the different spin state data, both before and after the polarization correction.
- "Display 4 XS" will show all 4 of the spin state data on a single panel for easy viewing. Only the polarization corrected data is shown. Note that the colors are scaled individually to each data set.
- Save State / Restore State allows you to export all of the parameters that you have entered in the table. This is a necessary step to save your work with the demo version of Igor. With the full version, saving the experiment will save the table automatically.

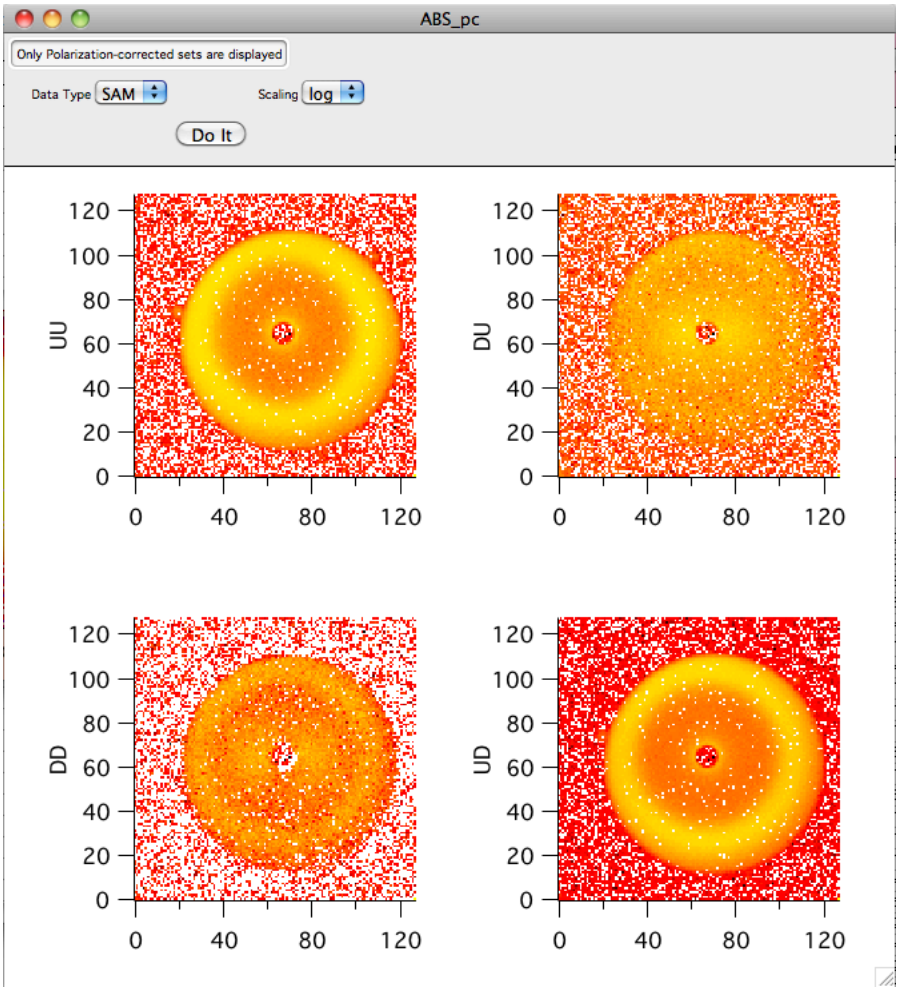
- NOTE - You'll need to repeat the steps of setting the files and the cells for each SAM, EMP, or BGD tab. You'll also need to repeat the Load and Pol Correct for each type of data, since each must be corrected on its own. -- Except for the BGD data, which is polarization independent. So simply enter the BGD scattering files as "UU". They're really used for all of the spin states.

- Once you've gotten all of the data files loaded and corrected, then the protocol is set up as usual, with the exception that you must save the protocol. "Reduce Data" will not use what is on the panel, but rather ask you for the name of the protocol that you what to use.

- Don't close the panel until you're done with the corrections or you'll lose what you've entered. Use the Macros Menu "Save State..." to save the run numbers that you've entered, and "Restore State..." to put them all back if you close the panel, or change to a different field condition. The menus options are found on the Macros Menu:



Display of 4 XS looks like this:



Other tidbits:

- Up to 10 files can be added together for each of the different spin states. This can be extended if needed.
- One polarization condition is set for everything with the popup @ the top.
- On loading of the data into the specified folder, the 2-letter spin state is tagged onto the loaded waves (all 4 of them). Then "_pc" is further tagged to the polarization corrected set.
- On loading, the raw files are added together as usual, normalized to monitor counts. Then each contribution of the file to the polarization matrix is added (scaling each by mon/1e8)
- Loaded data and PolMatrix are stored in the ususal SAM, EMP, BGD folders.
- Polarization correction is done with one click (one per tab). "_pc" tags are added to the resulting names, and copies of all of the associated waves are again copied (wasteful), but makes switching display very easy.
- Once all of the polarization correction is done, then the UU_pc (etc.) data can be reduced as usual (xx_pc = 4 passes, all done automatically).
- Protocol is built as usual, from this panel only (since the SAM, EMP, and BGD need to be switched as the reduction is repeated 4x, once for each spin state.
- Protocols can be saved/recalled as usual.
- However, reduction will always ask for a protocol rather than using what's on the panel.
- Export/Import of protocols is for Demo users. This saves the protocols to disk for later

import. Note that this does not include the file numbers for the EMP and BGD, since there are 4 XS. Use "Save State..." to save this information for later recall.

- Closing the panel will save the state (except the protocol). NOT initializing when re-opening will restore the state of the entered runs and the popups of conditions.

The math that is done here is:

$$\wp_{He} = P_o\, e^{-\Delta t/\Gamma}$$

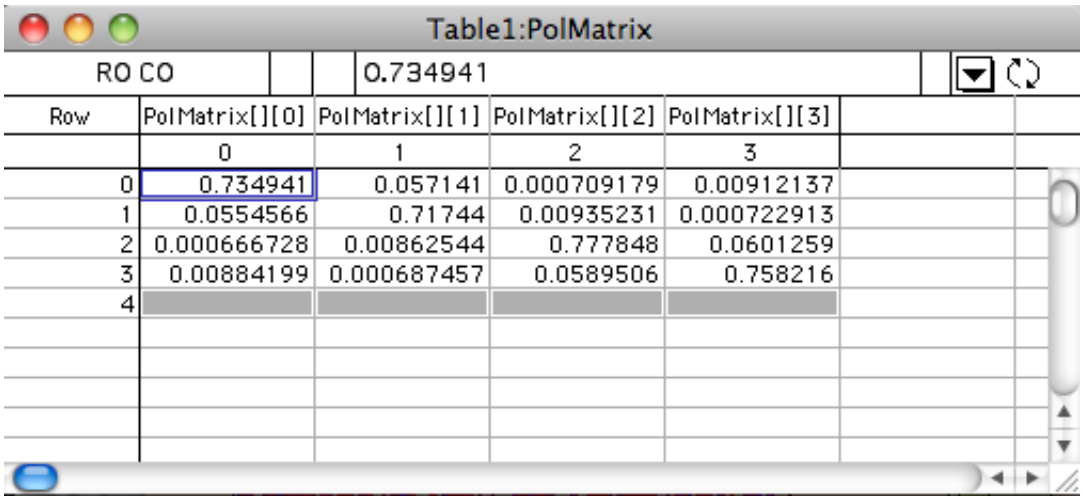
$$T_{maj} = T_e\, e^{-\mu(1-\wp_{He})}$$

$$T_{\min} = T_e\, e^{-\mu(1+\wp_{He})}$$

The results of Psm and PfPsm from the flipper panel (and the chosen field condition) are used here along with the major/minor transmissions. So then the elements of the 4x4 polarization matrix are:

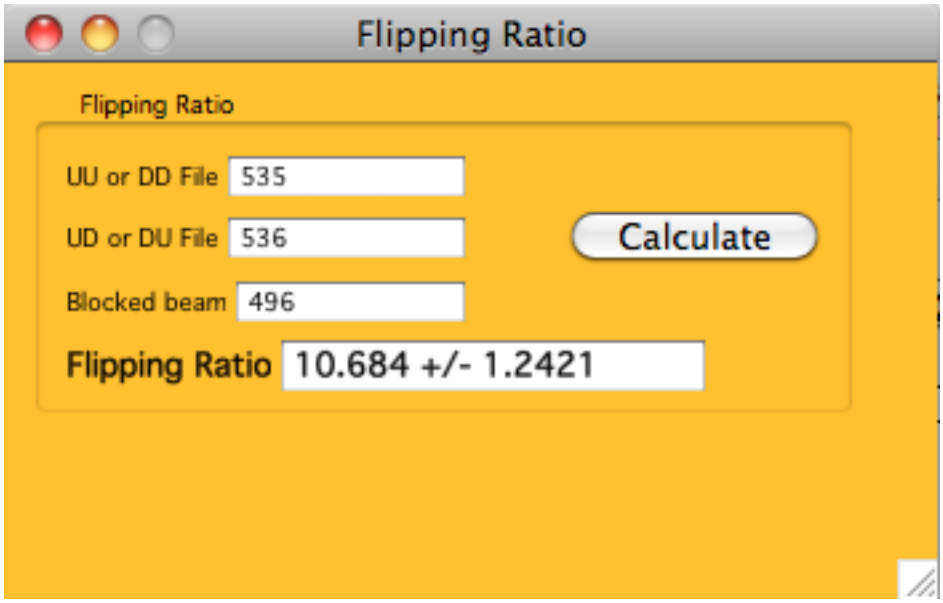
$$\begin{array}{lllll} UU: & (1+P_{sm})T_{maj} & (1-P_{sm})T_{maj} & (1-P_{sm})T_{\min} & (1+P_{sm})T_{\min} \\ DU: & (1-P_{sm}P_f)T_{maj} & (1+P_{sm}P_f)T_{maj} & (1+P_{sm}P_f)T_{\min} & (1-P_{sm}P_f)T_{\min} \\ DD: & (1-P_{sm}P_f)T_{\min} & (1+P_{sm}P_f)T_{\min} & (1+P_{sm}P_f)T_{maj} & (1-P_{sm}P_f)T_{maj} \\ UD: & (1+P_{sm})T_{\min} & (1-P_{sm})T_{\min} & (1-P_{sm})T_{maj} & (1+P_{sm})T_{maj} \end{array}$$

Then the polarization correction is done pixel-by-pixel, solving the system of linear equations for the (4) true cross sections. Clicking on "Show coef matrix" shows the coefficient matrix, its error, the inverse matrix, and its error. An example of the Polarization matrix is shown below, and may be useful for diagnostics if something just doesn't seem right.



Extra panel:

Flipping Ratio



From the Macros Menu, choose "Flipping Ratio"

Enter the run numbers for the transmission measurements for the specified spin states and the blocked beam, and the flipping ratio (and its uncertainty) are calculated. This value is not recorded anywhere or used for later calculations, but simply for information.
